MM 14: Topical Session Nanoanalytics using Small-Angle Scattering II

Time: Tuesday 11:45–12:45 Location: IFW A

Invited Talk MM 14.1 Tue 11:45 IFW A

Anomalous small-angle X-ray scattering in material science — •Armin Hoell — Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicker Strasse 100, 14109 Berlin, Germany.

Anomalous small-angle X-ray scattering (ASAXS) is an element-selective method based on the anomalous variation of the atomic scattering factor near absorption edges. Nowadays, ASAXS is a mature technique to analyse nano-structures as well as their chemical composition fluctuation. It is used in physics, chemistry, biology and soft / hard condensed matter. This talk will elaborate the advantages of ASAXS in the analysis of complex materials. In the first part important technical details and strategies to measure ASAXS will be emphasized. In the second part some material science applications are chosen to illustrate different aspects and benefits of ASAXS. While using the relative contrast variation between SAXS curves measured at different energies near below absorption edges of elements containing in the sample the composition fluctuations are derived in a demixed supercooled liquid state of a ZrTiCuNiBe alloy. The method of partial structure functions derived from ASAXS will be explained by way of the example of an AlNiLa alloy. So, in case of Ruthenium/Selenium based catalysts ASAXS allows to determine characteristic length-scales associated with three different structural elements. Furthermore, it will be shown how a simultaneous nonlinear regression method including physical constrains can be used to resolve the nano-structure of a silver-free photochromic glass.

MM 14.2 Tue 12:15 IFW A

Small Angle Scattering by Magnetic Nanoparticles — •Sabrina Disch, Raphaël P. Hermann, Peter Busch, Wiebke F. C. Sager, and Thomas Brückel — Institut für Festkörperforschung JCNS and JARA-FIT, Forschungszentrum Jülich GmbH; 52425 Jülich

Intensive research has been dedicated to magnetic nanostructures, both because of their possible applications, e. g. in medical imaging, catalysis, information storage, and owing to the interest in fundamental understanding of their magnetic properties. Magnetic nanoparticles, compared to bulk materials, show unique physical properties such as superparamagnetism or enhanced anisotropy constants. Very little is known about the magnetization distribution within a single particle and magnetic correlations in ordered arrangements of such nanoparticles. Small-angle scattering is the method of choice for investigating both intraparticular phenomena, such as the magnetization distribution or the spin structure of individual magnetic nanoparticles, and interparticular interactions of such nanoparticles in higher dimensional nanostructures. However, before addressing the problems of magnetization distributions or magnetic interactions between magnetic nanoparticles, the availability and the precise structural characterization of highly monodisperse nanoparticles is required. We developed a micellar synthesis route to cobalt nanoparticles with a narrow size distribution and will present latest advances in synthesis optimization and structural characterization along with recent work on highly monodisperse iron oxide nanospheres and nanocubes, including their deposition on substrates and structural characterization by SAXS and GISAXS.

MM 14.3 Tue 12:30 IFW A

Investigation of multiphase systems by small-angle scattering — •Dragomir Tatchev — Helmholtz Zentrum Berlin, Glienicker Str. 100, 14109 Berlin, Germany and Institute of Physical Chemistry - Bulgarian Academy of Sciences, Acad. G.Bonchev Str., Bl. 11, 1113 Sofia, Bulgaria

The two-phase approximation in small-angle scattering is well known and still dominating the data analysis. The intensity scattered at small angles is proportional to the second power of the difference between the scattering densities of the two phases. Simultaneously, scattering contrast variation techniques are widely used and they obviously target multiphase systems or systems with gradually varying scattering density since if no parasitic scattering contributions are present the scattering contrast variation would only change a proportionality coefficient. However, there are only scarce attempts to generalise the SAS theory for multiphase systems. Here we show that the scattered intensity at small-angles of a multiphase system can be presented as a sum of scattering of two-phase systems and terms describing interference between all pairs of phases. Extracting two-phase scattering patterns, called phase scattering functions, from multiphase samples by contrast variation is possible. These two-phase patterns can be treated with the usual SAS formalism. In the case of anomalous SAXS, the phase scattering functions have significant advantage over the partial structure factors since the later depend on all phases in the sample. The case of gradually varying scattering density is also discussed.

MM 15: Topical Session Nanoporous Functional Materials IV

Time: Tuesday 10:15–11:15 Location: IFW B

Topical Talk MM 15.1 Tue 10:15 IFW B

Fluidics with Nanoporous Solid-State Membranes: From Fundamental Physics to Applied Biology — •Patrick Huber — Faculty of Physics and Mechatronics Engineering, Saarland University, D-66041 Saarbrücken, Germany

Transport of fluids across nanopores plays a crucial role in phenomena ranging from clay swelling, frost heave, oil recovery and catalysis, to colloidal stability, protein folding and transport in cells and tissues. The advent of tailorable nano- and mesoporous membranes, most prominently arrays of carbon nanotube bundles, of silicon, silica and alumina channels, has led to a growing interest in fundamental and applied questions with regard to the transport phenomenology across this kind of nanostructures. After a short introduction into this sub-field of nanofluidics, I will present experiments on pressure-driven and self-propelled (capillarity-driven) transport of fluids in nanochannels and will highlight differences between nanoscopic and macroscopic transport principles. Finally, I will elucidate how protein translocation experiments across artificial nanochannel arrays may allow the exploration of the transport machinery at biomembranes.

MM 15.2 Tue 10:45 IFW B

Crystallization Kinetics Dictate the Molecular Arrangement in Nanochannels — •Anke Henschel, Klaus Knorr, and Patrick Huber — Saarland University, Saarbruecken, Germany

We present an x-ray diffraction study on the crystallization of chain-like molecules (medium length n-alkanes and n-alcohols) in arrays of lined up, tubular silicon and silica channels (mean channel diameters of 10 nm)[1–2].

The samples, prepared by capillary condensation or filling in the liquid state and subsequent cooling below the pore freezing point, exhibit diffraction patterns typical of significant, anisotropic orientation distributions of the pore crystals. The architectural principle common to all observed textures originates in a nano-scale version of the mechanism underlying the Bridgman technique of single crystal growth: Upon solidification of completely filled nanochannels the fastest, and hence dominant growth direction, propagates along the long axes of the channels and thereby dictates a distinct orientational arrangement of the molecular crystals.

(1) A. Henschel, T. Hofmann, P. Huber, K. Knorr, Phys. Rev. E 75, 021607 (2007).

(2) A. Henschel, P. Huber and K. Knorr, Phys. Rev. E 77, 042602 (2008).

MM 15.3 Tue 11:00 IFW B

Electrostatic Doping of Strongly Correlated Systems — •Ajay Kumar Mishra, Azad Darbandi, Robert Kruk, and Horst Hahn — Institute for Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany

We present a study on the tuneable magnetic transitions using electrostatic doping (electrostatic modulation of the carrier density upon

surface charging). In strongly correlated materials, like colossal magnetoresistance compounds (CMR), electrostatic doping can alter fundamental properties of the electronic system by inducing phase transitions.

Since the electrostatic doping is a surface effect a large surface-to-volume ratio is desired to get an appreciable modification of the physical properties. In order to obtain such nanostructures, La1-xSrxMnO3 (LSMO) nanoparticles were synthesized by spray pyrolysis. The microstructure of the as synthesized nanoparticles consists of porous, shell-like structures with a particle size of about 8 nm. The magnetic measurements of nanoparticles show superparamagnetic behavior at room temperature. A controlled post annealing was carried out to bring the ferromagnetic transition slightly above room temperature. The sharp transition and favorable surface-to-volume ratio is reached at annealing temperatures between 800-1100 0C, resulting in grain sizes ranging from 30 to 80 nm. A reversible change of 2 % in magnetization is observed when the charge is applied at the solid-electrolyte interface. The magnetization modulation upon charging is discussed in terms of the reversible electrostatic hole doping.

MM 16: Diffusion and Point Defects I

Time: Tuesday 11:30–12:30 Location: IFW B

MM 16.1 Tue 11:30 IFW B

Diffusion and Crystallization in Magnetron Sputtered SiC Films — •Wolfgang Gruber and Harald Schmidt — TU Clausthal, Institut für Metallurgie, AG Materialphysik

Thin films of amorphous and polycrystalline SiC have a great potential for applications in various branches of technology. For a tailored production of polycrystalline films a understanding of nucleation and growth mechanisms which determine the microstructure are necessary. X-ray diffractometry (XRD) and transmission electron microscopy (TEM) studies on r.f. co-sputtered SiC films yielded a strong dependence of the crystallization rates on the substrate. For single crystalline silicon as a substrate an activation energy of about 4 eV is found for the rate of crystallization. If glassy carbon is used as a substrate the corresponding activation energy is about 9 eV. For a closer investigation of this phenomenon, in this study we investigated films deposited on different substrates with different thickness (100 nm to 1000 nm) and variable composition SiCx. Since self-diffusion plays an important role for crystallization we measured the diffusivities of the constituting elements using isotope enriched heterostructures and secondary ion mass spectrometry (SIMS). Based on the experimental results a model for crystallization kinetics is discussed.

MM 16.2 Tue 11:45 IFW B

Atom Jumps Studied by Coherent Synchrotron Radiation — •Gero Vogl[1], Michael Leitner[1], Bastian Pfau[2], Bogdan Sepiol[1], and Lorenz-Mathias Stadler[1] — [1]Fakultät für Physik der Universität Wien, Austria — [2]BESSY, Berlin, Germany

Measuring the atomic diffusion jump is a fundamental problem in solid state physics. Up to now only measurements involving a limited number of isotopes and in a very limited temperature range were feasible due to the limitations of methods such as quasi-elastic neutron scattering, quasi-elastic Mössbauer spectroscopy or nuclear magnetic resonance.

X-ray photon correlation spectroscopy has the potential to overcome these constraints. We present the first successful implementation of this new technique. We deduce the atomic jump model from the q-dependent relaxation times of diffuse scattering measured at the ESRF and give the activation energy of Au diffusion in CuAu. We predict that the new sources with increased brilliance and high coherence like PETRA or the XFEL will enable determination of the atomic diffusion jump in condensed matter over a wide range.

MM 16.3 Tue 12:00 IFW B

Self-diffusion in Germanium at Low Temperatures — •Erwin Hüger[1], Ursula Titze[2], Dieter Lott[2], Hartmut Bracht[3], Dominique Bougeard[4], Eugene E. Haller[5], and Harald Schmidt[1] — [1]TU Clausthal, Germany — [2]GKSS Forschungszentrum Geesthacht, Germany — [3]Universität Münster, Germany — [4]TU München, Germany — [5]University of California at Berkeley, USA

Self-diffusion in intrinsic single crystalline germanium was investigated between 429 and 596 °C using ^{70}Ge/^{nat}Ge isotope multilayers. The diffusivities were determined by neutron reflectometry from the decay of the first and third order Bragg peak. At high temperatures the diffusivities are in excellent agreement with literature data obtained by ion beam sputtering techniques, while considerably smaller diffusion lengths between 0.6 and 4.1 nm were measured. At lower temperatures the accessible range of diffusivities could be expanded to values $D < 1 \times 10^{-25}$ m^{2}s^{-1} which is three orders of magnitude lower than the values measured by sputtering techniques. Taking into account available data on Ge self-diffusion, the temperature dependence is accurately described over nine orders of magnitude by a single Arrhenius equation. An activation enthalpy of diffusion of (3.13 ± 0.03) eV and a pre-exponential factor of 2.54×10^{-3} m^{2}s^{-1} for temperatures between 429 and 904 °C are obtained. Single vacancies are considered to prevail self-diffusion in Ge over the whole temperature range.

MM 16.4 Tue 12:15 IFW B

Defect structures in CaF_2 for optical applications — •Stephan Rix[1,2], Marisa Aigner[1], Claudia Felser[2], Martin Letz[1], Ute Natura[3], and Lutz Parthier[3] — [1]Schott AG, Mainz — [2]Johannes Gutenberg-Universität, Mainz — [3]Schott Lithotec, Jena

Single crystal calcium fluoride (CaF_2) is an important lens material for deep-ultraviolet optics used in microlithographic structuring of semiconductors. High radiation densities require an extreme laser-stability of the material. The quality of the material strongly depends on a high purity level. For long exposure times the optical quality of CaF_2 is affected by radiation-induced defect structures, namely F- and H-centers. The migration and agglomeration of these defect structures play an important role in understanding laser-damage processes on a microscopic level. We use ab-initio methods to investigate the stabilization of laser-induced defects by agglomeration or impurities. As stabilization processes involve defect migration, we also focus on diffusion properties of defects. We present a method for the calculation of diffusion barriers, which shows good agreement with experimental results for the F-center with well localized electronic wave functions.

MM 17: Mechanical Properties III

Time: Tuesday 10:15–11:45 Location: IFW D

MM 17.1 Tue 10:15 IFW D

Change of deformation mechanism in nanocrystalline nickel at very low temperatures — •Lutz Hollang, Suhash Ranjan Dey, and Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden

Pure nanocrystalline nickel was produced by pulsed electro-deposition without additives for grain refinement. The average grain size of the material is d(EBSD) = 150 nm and d(XRD) = 25 nm if determined by electron backscatter diffraction (EBSD) and X-ray diffraction (XRD), respectively. Tensile tests with constant deformation rate were performed at temperatures between 4 K and 320 K. The stress-strain curves are parabolic with the ultimate stress strongly decreasing with increasing temperature. Stress relaxation experiments reveal that dislocation interaction governs the plastic behaviour of the material at low temperatures. However, if the stress reaches the threshold of 2400 MPa, as it is the case between 4 K and 9 K, the deformation mode suddenly changes towards ‘catastrophic‘ shear. The shear events are characterized by substantial stress drops accompanied by acoustic